An Influence of the Elastic Properties of Composite Components on the Mechanical Response of Polycrystalline Structures at Yield Level

Tomasz Sadowski and Eligiusz Postek

Abstract The aim of this paper is to present a constitutive model in the case of an uniaxial tension of the polycrystalline materials including the inter-granular metallic layers, creating its internal structure. The paper is focused on the discussion of the elastic properties of a composite components influence on the overall material response. The effective continuum model was applied to get the constitutive relations. Representative Volume Element (RVE) was analysed taking into consideration an initial internal structure of the material obtained from SME photographs. Owing to a high complexity of the internal structure of the composite material, FEA technique was used to get macroscopic stress-strain correlations. They include gradual changes of the internal structure of the material due to porosity and cracks development under tension.

Keywords Polycrystalline ceramics · inter-granular layers · different elastic properties of components

1 Introduction

Ceramic polycrystalline composites have a non-linear and complex response to applied loads due to their internal structure. Experimental observations show that the most important element of the internal structure is the thin layer between grains. The size of these layers is relatively small in comparison to the grain diameter. These composites can be treated as two-phase materials. The inter-granular layers can significantly change the macro-response of the material. This is particularly evident when the two phases are made of different materials. For example, the grains may be brittle but the thin layers exhibit properties of a metallic material, so the softening effect due to porosity development should be taken into account. Micropores act as stress concentrations and locally change the state-of-stress, leading to

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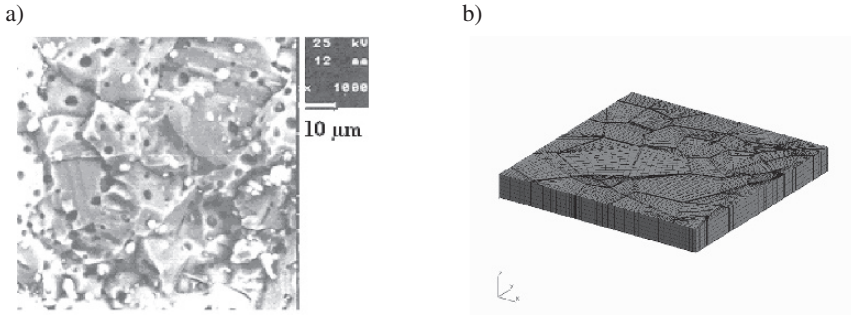ul. Nadbystrzycka 40, 20–618 Lublin, Poland
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a)   b)

Fig. 1 SEM photograph: (**a**) fracture surface of polycrystalline ceramics, (**b**) FEA model (RVE)

the development of cracks. Experimental results show that defects develop mainly inter-granularly and cause in-homogeneity and induced anisotropy of the solid.

The paper is focused on the discussion of the elastic properties of a composite components influence on the overall material response. Modelling of such a material response is possible by the application of effective continuum models. Representative Volume Element (RVE) was analysed by taking into consideration an initial internal structure of the material obtained from SME photographs, Fig. 1. Owing to a high complexity of the internal structure of the composite material, FEM technique was used to get macroscopic stress-strain correlations.

2 Formulation of the Problem

Let us consider a composite made of elastic grains (e.g. Al_2O_3) and visco-plastic inter-granular phase (e.g. Co). In order to investigate of the material response at yield limit, assume that the composite is subjected to uniaxial tension and that strains (observable in experiments) are small. Let us consider RVE, i.e. the smallest part of the composite that can accurately represent the macroscopic material response. In comparison to [1] and [2] in this paper a discussion of the: (1) initial elastic properties and (2) level of porosity in interfaces on the composite behaviour was done.

2.1 Elastic and Plastic Properties of a Composite Components

Denoting by $\bar{V}^{(1)}$ the volume fraction of elastic grains in RVE and by $\bar{V}^{(2)}$ the volume fraction of visco-plastic interfaces one can estimate the averaged properties of two-phase composite with application of the linear rule of mixture (RoM),

$$P^{\text{av}} = P^{(1)}\bar{V}^{(1)} + P^{(2)}\bar{V}^{(2)} \tag{1}$$

where $P^{(1)}$ and $P^{(2)}$ correspond to the properties of grains and interface, respectively.

In the considered two-phase composite the initial porosity could appear in both parts of the composite components, i.e. in elastic grains and along interfaces. Let us assume that the initial porosities are uniformly distributed in both phases independently. Then, the effective elastic moduli of solids with non-interacting cavities could be expressed according to [3]:

$$E^{\text{eff}}/E_0 = 1/(1+3p); \qquad \nu^{\text{eff}} = 1/3 + (\nu_0 - 1/3)(1+3p) \qquad (2)$$

where p denotes: grains porosity $p^{(1)}$ or inter-layer porosity $p^{(2)}$. Figure 2 shows distribution of the effective moduli in relation to material porosity p. It is necessary to emphasize that application of linear RoM approach to estimate the porous effective properties is not enough, because of high nonlinearity. If any phase contains initial porosity, then effective elastic properties were estimated according to (2) and then introduced to (1) to estimate averaged composite properties.

The basic mechanical properties used in numerical examples were summarized in Table 1.

We have assumed the volume fraction of grains as equal to $\bar{V}^{(1)} = 0.9029$, whereas corresponding volume fraction of inter-layers – $\bar{V}^{(2)} = 0.0971$.
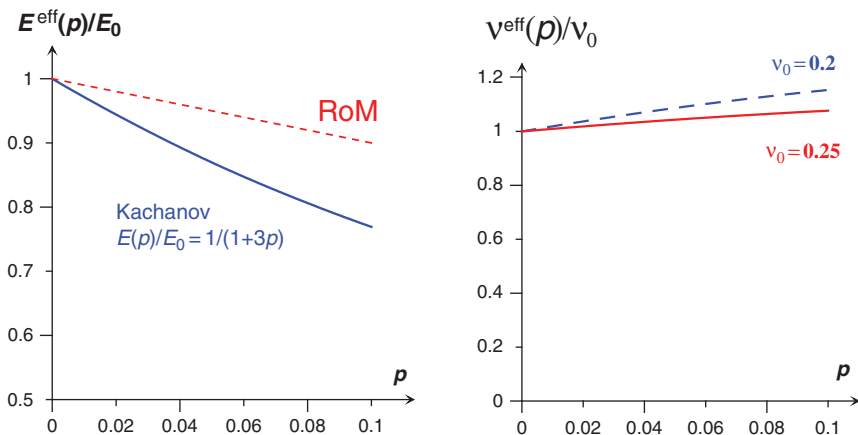

Fig. 2 Distribution of effective moduli in relation to material porosity p

Table 1 The basic mechanical properties of the grains (phase 1) and inter-layers (phase 2)

Mechanical property	Grains (phase 1)	Inter-layers (phase 2)
Young modulus	$E_{(1)} = 410\,\text{GPa}$	$E_{(2)} = 210\,\text{GPa}$
Poisson ratio	$\nu_{(1)} = 0.25$	$\nu_{(2)} = 0.235$
Yield limit		$\sigma_y^{(2)} = 297\,\text{MPa}$
Fluidity parameter		$\gamma_{(2)} = 10^{-10} - 10^{-5}/(\text{MPa s})$

2.2 Basic Equations

To solve the problem of the polycrystalline composite response it is necessary to describe visco-elastic-plastic behaviour of the inter-granular layers. According to [4], the total strain rate can be split into elastic part $\dot{\varepsilon}_{ij}^{e}$ and visco-plastic one $\dot{\varepsilon}_{ij}^{v-p}$

$$\dot{\varepsilon}_{ij} = \dot{\varepsilon}_{ij}^{e} + \dot{\varepsilon}_{ij}^{v-p} \tag{3}$$

If the elastic properties of the material are defined by the elasticity matrix D_{ijkl}, then one can find the total stress rate $\dot{\sigma}_{ij}$

$$\dot{\sigma}_{ij} = D_{ijkl}\dot{\varepsilon}_{kl}^{e} \tag{4}$$

When the yield condition is satisfied $F(\sigma_{ij}, \varepsilon_{kl}^{v-p}) = F_0$, visco-plastic behaviour of the material occurs and the inelastic strains appears in part of the material, i.e. inter-granular layers if

$$F(\sigma_{ij}, \varepsilon_{kl}^{v-p}) > F_0 \tag{5}$$

F_0 denotes the uniaxial yield stress. In the general case of non-associated plasticity theory, the visco-plastic strain rate can be defined in the following form

$$\dot{\varepsilon}_{ij}^{v-p} = \gamma \langle \varphi(F) \rangle \frac{\partial Q}{\partial \sigma_{ij}} \tag{6}$$

where Q denotes the plastic potential, γ is the fluidity parameter related to the plastic flow rate and the function $\langle \varphi(F) \rangle$ is given by

$$\langle \varphi(F) \rangle = \begin{cases} 0 & \text{for} \quad F \leq F_0 \\ \varphi(F) & \text{for} \quad F > F_0 \end{cases} \tag{7}$$

as well as

$$\varphi(F) = \exp[M(F - F_0)/F_0] - 1 \tag{8}$$

where M is a constant describing the particular plastic behaviour of the material. For associative plasticity theory, $F = Q$ and the constitutive equation (6) takes the form

$$\dot{\varepsilon}_{ij}^{v-p} = \gamma \langle \varphi(F) \rangle \frac{\partial F}{\partial \sigma_{ij}} \tag{9}$$

In order to get the strain increment $\Delta\varepsilon_{ij}^{v-p(n)}$ it is necessary to define a time increment $\Delta t^{(n)} = t^{(n+1)} - t^{(n)}$ for two neighbouring times. Then the strain increment is equal to

$$\Delta\varepsilon_{ij}^{\text{v-p(n)}} = \Delta t^{(n)}[(1 - \Theta)\dot{\varepsilon}_{ij}^{\text{v-p(n)}} + \Theta\dot{\varepsilon}_{ij}^{\text{v-p(n+1)}}] \tag{10}$$

when a trapezium rule is applied. Θ is the parameter depending on the chosen time integration rule.

The visco-plastic strain rate $\dot{\varepsilon}_{ij}^{\text{v-p(n+1)}}$ for the time of the loading process $t^{(n+1)}$ is equal to [4]

$$\dot{\varepsilon}_{ij}^{\text{v-p(n+1)}} = \dot{\varepsilon}_{ij}^{\text{v-p(n)}} + H_{ijkl}^{(n)}\Delta\sigma_{kl}^{(n)} \tag{11}$$

and the matrix $H_{ijkl}^{(n)}$ is expressed by

$$H_{ijkl}^{(n)}(\sigma_{kl}^{(n)}) = \left(\frac{\partial\dot{\varepsilon}_{ij}^{\text{v-p}}}{\partial\sigma_{kl}}\right)^{(n)} \tag{12}$$

Introducing equation (11) to (10) gives

$$\Delta\varepsilon_{ij}^{\text{v-p(n)}} = \dot{\varepsilon}_{ij}^{\text{v-p(n)}}\Delta t^{(n)} + C_{ijkl}^{(n)}\Delta\sigma_{kl}^{(n)} \tag{13}$$

where

$$C_{ijkl}^{(n)} = \Theta\Delta t^{(n)} H_{ijkl}^{(n)} \tag{14}$$

The stress increment can then be calculated according to the following rule

$$\Delta\sigma_{ij}^{(n)} = D_{ijkl}^{(n)}(\Delta\varepsilon_{kl}^{(n)} - \Delta\varepsilon_{kl}^{\text{v-p(n)}}) \tag{15}$$

or alternatively

$$\Delta\sigma_{ij}^{(n)} = \hat{D}_{ijkl}^{(n)}(\Delta\varepsilon_{kl}^{(n)} - \dot{\varepsilon}_{kl}^{\text{v-p(n)}}\Delta t^{(n)}) \tag{16}$$

where the matrix describing the material properties is equal to

$$\hat{D}_{ijkl}^{(n)} = (I_{ijtw} + D_{ijrs}C_{rstw}^{(n)})^{-1}D_{twij} = (D_{ijkl}^{-1} + C_{ijkl}^{(n)})^{-1} \tag{17}$$

The increment of nodal displacements can be calculated knowing the tangential stiffness matrix $K_{sm}^{\text{T(n)}}$ and the increase of the "so called" vector of pseudo-load $\Delta V_m^{(n)}$, [4]

$$\Delta u_s^{(n)} = [K_{sm}^{\text{T(n)}}]^{-1}\Delta V_m^{(n)} \tag{18}$$

Having defined problem incrementally, e.g. (13), (16) and (18), one can calculate the current values of strain, stress and displacement for the time while $t^{(n+1)}$.

2.3 Yield Conditions for Non-Hardening Material Without and with Porosity

If the material does not contain any initial porosity and non-hardening effects, we assume that its behaviour could be described by the following yield condition

$$F(\sigma_{sm}) = \sqrt{3J'} = \sqrt{(3/2)\sigma'_{sm}\sigma'_{sm}} = \sigma_y^{(2)} \tag{19}$$

where $\sigma_y^{(2)}$ is the yield stress of the plastic inter-layers and σ'_{sm} denotes the stress deviator. For material with initial porosity of volume content $p^{(2)}$ we adopt Gurson-Tvergaard yield condition [5, 6]

$$F = \left(\frac{\sigma^M}{\bar{\sigma}}\right)^2 + 2q_1 p^{(2)} \cosh\left(\frac{3q_2\sigma_m}{2\bar{\sigma}}\right) - \left(1 + q_3[p^{(2)}]^2\right) \tag{20}$$

where σ^M is the Huber – von Mises stress, σ_m is the mean stress, $\bar{\sigma}$ is the Huber – von Mises stress in the matrix (i.e. in inter-layers) and q_1, q_2, q_3 are the Tvergaard coefficients. The detailed analysis for different $p^{(2)}$ values has been performed in [7].

3 Numerical Examples

For investigations of the elastic properties influence of the composite phases 1 and 2 on the purely elastic polycrystalline composite behaviour, the RVE (Fig. 1) was subjected to uniform tension along direction x. To analyse weaker properties of inter-layers in comparison to grains the following variation of $E_{(1)}/E_{(2)} = 10$, 5 and 1 were taken into account (assuming $E_{(1)} = 410$ GPa). For the remaining ratios $E_{(1)}/E_{(2)} = 1/5$ and $1/10$ (with $E_{(2)} = 410$ GPa) weaker grains in comparison to interfaces were investigated. Comparing Figs 3 and 4 one can notice highly diverse displacement distribution for both considered limiting cases. For homogeneous ma-
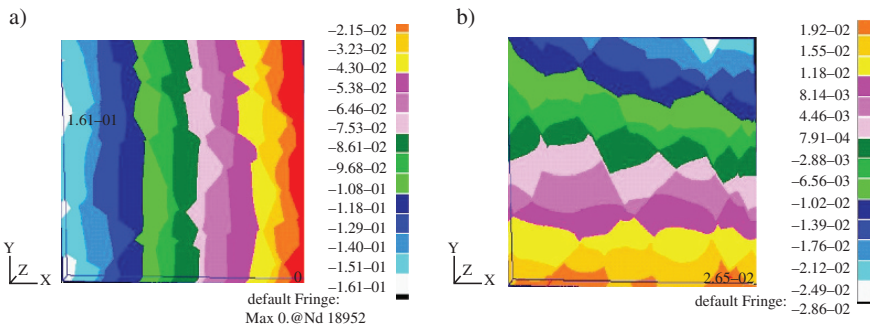

Fig. 3 Displacement along: (**a**) tensile direction u_x and (**b**) perpendicular direction u_y for $E_{(1)}/E_{(2)} = 10$
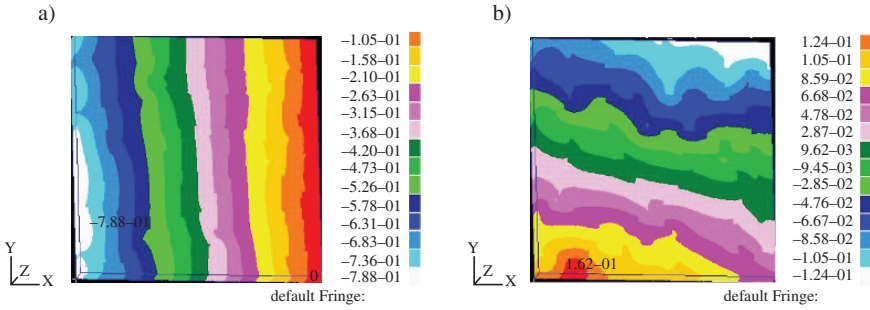
Fig. 4 Displacement along: (**a**) tensile direction u_x and (**b**) perpendicular direction u_y for $E_{(1)}/E_{(2)} = 1/10$

terial ($E_{(1)} = E_{(2)} = 410\,\text{GPa}$) appropriate distributions are: regular vertical (u_x) or horizontal strips (u_y). As it was expected, the deformations of RVE are much higher in case of composite with weaker grains, Fig. 5. If the inter-layers have significantly less elastic modulus in comparison to grains, u_y^{max} does not change substantially. Figure 5 presents also the influence of the initial porosity of the inter-faces ($p^{(2)}$) on the RVE response. This phenomenon has a great importance in case of composites with weak grains (left part of the plot). Figures 6 and 7 specify differences in stresses distributions: σ_{xx} and σ_{yy} for both considered limiting cases. For homogeneous material ($E_{(1)} = E_{(2)} = 410\,\text{GPa}$) they are uniform and $\sigma_{xx} = 400\,\text{MPa}$ and

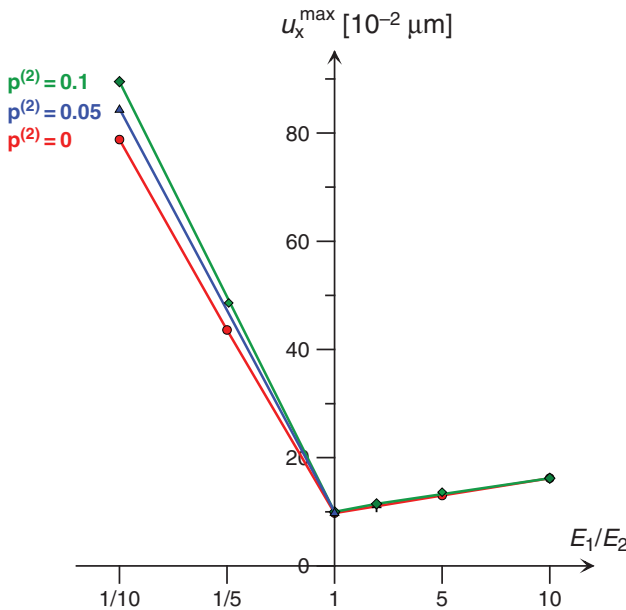**Fig. 5** Maximum displacement u_x in RVE for different ratios $E_{(1)}/E_{(2)}$

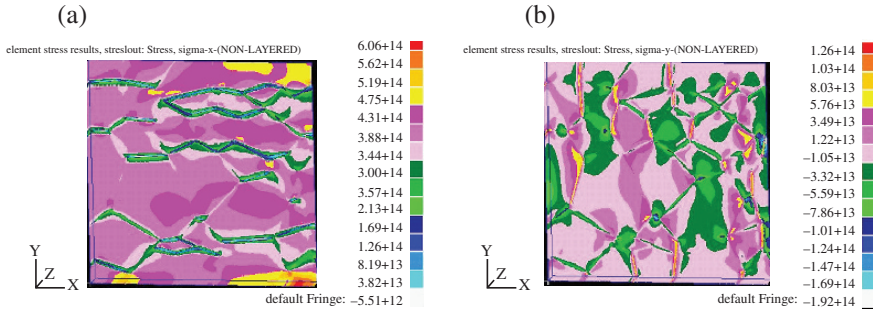(a)   (b)

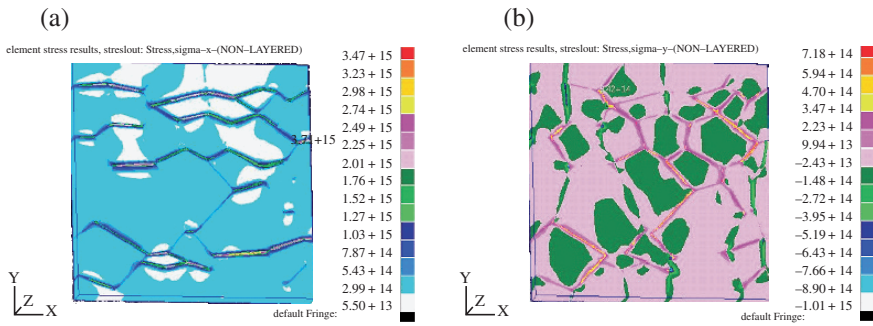**Fig. 6** Stress distribution for $E_{(1)}/E_{(2)} = 10$: (**a**) σ_{xx} and (**b**) σ_{yy}

(a)   (b)

Fig. 7 Stress distribution for $E_{(1)}/E_{(2)} = 1/10$: (**a**) σ_{xx} and (**b**) σ_{yy}

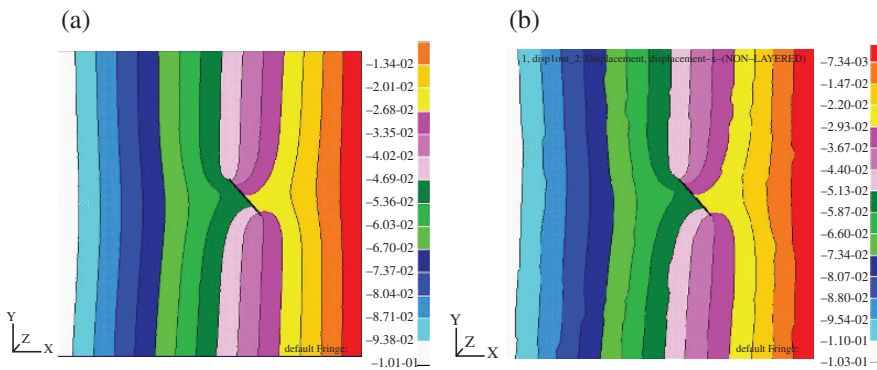(a)   (b)

Fig. 8 Displacement u_x distribution for: (**a**) $E_{(1)}/E_{(2)} = 1$ (elastic continuum) and (**b**) $E_{(1)}/E_{(2)} =$ 1.95 and plastic behaviour of the inter-layers, Table 1
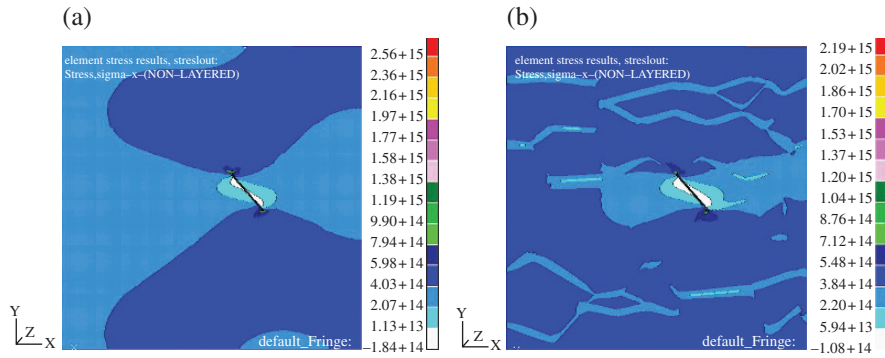
Fig. 9 Stress distribution σ_{xx} for: (**a**) $E_{(1)}/E_{(2)} = 1$ (elastic continuum) and (**b**) $E_{(1)}/E_{(2)} = 1.95$ and plastic behaviour of the inter-layers, Table 1

$\sigma_{yy} = -206$ MPa. Then the σ_{xx} stress concentration for case $E_{(1)}/E_{(2)} = 10$ is equal to 1.626, whereas for $E_{(1)}/E_{(2)} = 1/10 - 9.275$.

If in the composite appears straight crack, then the displacement of RVE is totally different. Figure 8a shows displacement distribution for purely elastic RVE ($E_{(1)} = E_{(2)} = 410$ GPa), whereas in Fig. 8b both phases are described according to Table 1. Due to inter-layers the maps of displacements are not smooth and the maximum displacement is 8.91% higher in the second case.

One can observe also differences in stress distributions in two considered examples due to inter-layers presence, Fig. 9. The stress concentrations appear at the discontinuity tips and its growth could be along inter-layers.

4 Conclusions

The presented results established the influence of the elastic component properties in polycrystalline composite material on the total macroscopic response. The presence of the initial porosity will significantly increase all deformation characteristics of the composite material. The occurrence of cracks in a polycrystalline structure which contains visco-plastic inter-layers will significantly change the stress and displacement distributions causing local stress concentrations and further crack growth. The obtained results could be useful for engineers who are introducing new technological approaches to the modeling of modern composite materials for special applications in order to get desired macro-properties of the composite using data concerning their components.

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